RAMAN SPECTROSCOPY OF STRUCTURALLY RELATED CHEMICALLY SUBSTITUTED CARBOHYDRATES: X-FLUORO-X-DEOXY-D-GLUCOSE MOLECULES

J. P. Ryall[1], R. Withnall[1]*, T. J. Dines[2] and B. Z. Chowdhry[1*]

[1]Vibrational Spectroscopy Centre, School of Sciences, University of Greenwich, Medway Campus, Pembroke, Chatham Maritime, Kent ME4 4TB, UK; E-Mail: b.z.chowdhry@gre.ac.uk
[2]Division of Physical and Inorganic Chemistry, Carnelley Building, University of Dundee, Dundee DD1 4HN, UK

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Abstract: The Raman spectra of protonated and deuteriated powder samples of α-D-glucose, 2-deoxy-D-glucose, 2-fluoro-2-deoxy-D-glucose, 3-fluoro-3-deoxy-D-glucose and 6-fluoro-6-deoxy-D-glucose have been examined. In addition a*b initio* calculations of the molecular structures of the aforementioned molecules and their associated vibrational modes have been conducted using the hybrid SCF-DFT (B3-LYP) method incorporating a cc-pVDZ basis set.

Fluoro- analogues of deoxy-D-glucose are the main subject of this study and include 2-fluoro-2-deoxy-D-glucose, 3-fluoro-3-deoxy-D-glucose and 6-fluoro-6-deoxy-D-glucose where the labile proton at the designated position (C-2, C-3 or C-6) is substituted with a fluorine atom. Both 2-fluoro-2-deoxy-D-glucose and 3-fluoro-3-deoxy-D-glucose have fluorine atoms on the hemiacetal ring whereas 6-fluoro-6-deoxy-D-glucose has a fluorine atom on the C-6 of the CH_2 group. 2-Fluoro-2-deoxy-D-glucose is used in clinical medicine in its isotopically labelled form (^{18}FDG), as a metabolic marker for positron emission tomography (PET) imaging [1]. However the impetus for conducting this study is two fold: an inherent knowledge base reasoning and also because there is a lack of data in the scientific literature concerning the relationship between molecular structures of chemically substituted monosaccharides and their vibrational spectroscopic properties.

The Raman spectra of protonated and deuteriated samples of 2-fluoro-2-deoxy-D-glucose and 6-fluoro-6-deoxy-D-glucose, obtained using a laser exciting wavelength equal to 632.8 nm, are shown in Fig. 1a and 1b respectively. Comparisons of the protonated and deuteriated samples show that full deuteriation has taken place. The Raman spectral profiles of the 2-fluoro-2-deoxy-D-glucose and 6-fluoro-6-deoxy-D-glucose are quite different in the spectral region shown.

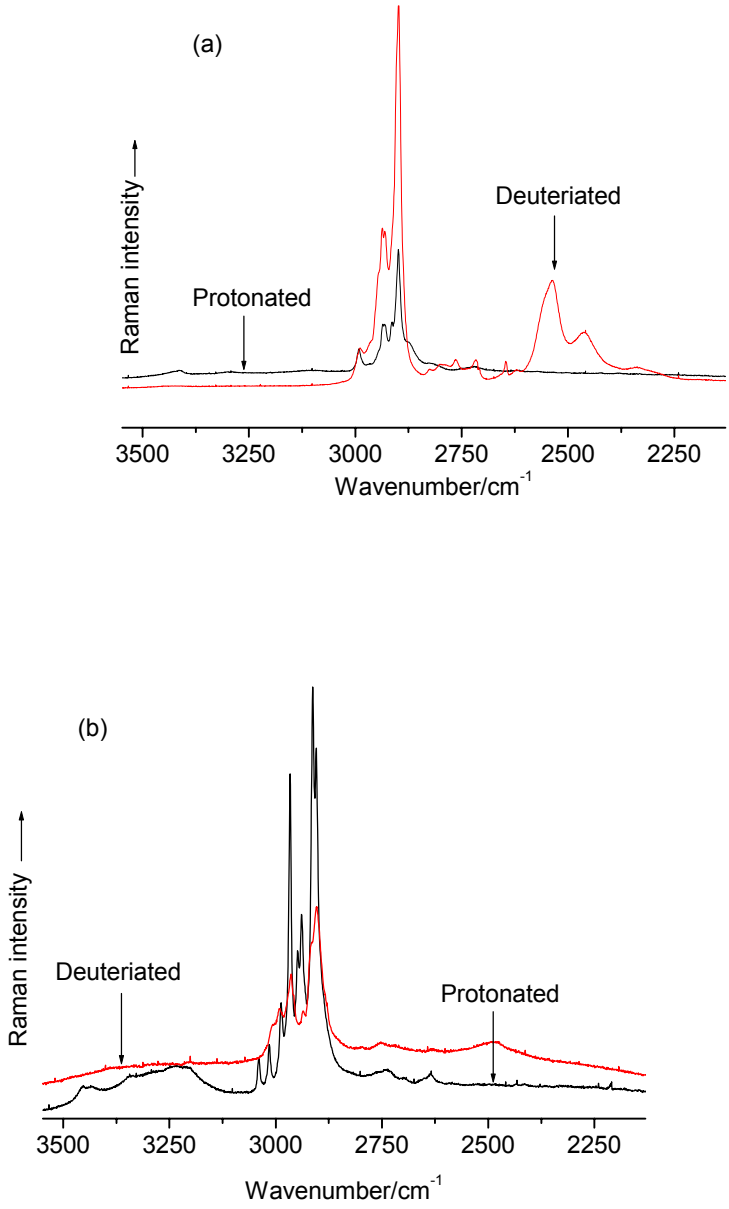

Fig. 1. Raman spectra of (a) 2-fluoro-2-deoxy-D-glucose and (b) 6-fluoro-6-deoxy-D-glucose.

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References:

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